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Study of Si-based three-dimensional photonic crystals infiltrated with liquid crystal within a one-dimensional effective model

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In this work, we study Si-based three-dimensional photonic crystals infiltrated with liquid crystal (LC), within a one-dimensional effective medium model. Two specific systems of diamond crystal structure compatible with the mature Si technology are considered, namely, (i) diamond-1 which is composed of LC spheres embedded in the Si background, and (ii) diamond-2 which is the inverse of the foregoing structure, with Si spheres immersed in the LC background. For each system, the study is carried out with the LC being in the isotropic/nematic phase. The one-dimensional effective medium model employed in the study is an improved version of the conventional mean field theory (MFT). While retaining partially the typical advantage of MFT, e.g., physical transparency, analytical capability, and computational efficiency, it goes beyond the conventional MFT by taking into account the modulation of dielectric constant in the direction of wave propagation. As such, it improves greatly the poor numerical accuracy inherent in the MFT. We find a partial gap between the 2nd and 3rd bands, with the gap-to-midgap ratio being a few percents. Moreover, the edge of partial gap may be shifted by about 1% (in relative unit) when optical, thermal, or electrical means are applied to alter the phase of LC or rotate the axis of nematic molecules. © 2011 American Institute of Physics. [doi:10.1063/1.3603008]

I. INTRODUCTION

Photonic crystals (PCs) are man-made crystals with periodically varying profiles of refractive index to modulate light propagation for important photonic applications.^{1–4} In such systems, the wave propagation is strongly affected by the Bragg scattering $\mathbf{k} \rightarrow \mathbf{k}' = \mathbf{k} - \mathbf{G}$, where $\mathbf{k}$ = wave vector and $\mathbf{G}$ = reciprocal lattice vector, which results in pronounced modification in the dispersion relation $\omega(\mathbf{k})$ and creates frequency gaps called photonic band gaps (PBGs) similar to electronic energy gaps of crystals in solid state physics. At a gap frequency, the wave propagation is forbidden and the photon can be localized. Apart from PBGs, a typical photonic band structure also shows other features commonly seen in electronic band structures, such as zero or even negative group velocities. Based on these features, numerous photonic applications can be realized, for example, wave guides,^{5,6} waveguides with semislow light and tailored dispersion properties,⁷ or nanocavities for ultrafast lasers.⁸

One focus in the field is the search for three-dimensional (3D) PCs with tunable PBGs. 3D PBGs provide better light confinement than two-dimensional (2D) PBGs in the application of waveguides, and the tunability gives PCs the additional device potential as light switch/modulators. In general, it is difficult to find full PBGs in 3D PCs because of band degeneracy at high symmetry points of the Brillouin zone, although phenomenal success has been achieved, for example, in the case of diamond structure.^{9,10} Li *et al.* have

discussed the idea of lifting the degeneracy by introducing anisotropic dielectric materials into PCs. They report the opening of partial gaps in cubic PCs composed of optically birefringent tellurium (Te) spheres, which can be used to filter the light propagating in a range of solid angle with respect to the extraordinary axis of Te spheres.¹¹ Busch and John have proposed an inverse opal PC of face-centered cubic (FCC) structure infiltrated with nematic liquid crystal (LC).¹² They have shown that a full PBG exists between the 8th and 9th bands and is completely tunable with an electric field which rotates the orientation of nematic molecules. On the other hand, liquid crystals can also be switched, by thermal or optical means, between isotropic (disordered) and nematic (ordered) phases and exhibit different refractive properties.^{13–15} Together, electrical, thermal, and optical tuning of the dispersion in 1D, 2D, and 3D PCs infiltrated with LCs^{16–18} have now emerged as an important field in the new area of optofluidics.

The present work investigates the structure of a 3D Si-based PC infiltrated with liquid crystal, which has the feature of being compatible with the present mature semiconductor technology and, hence, useful for the realization of photonic integrated circuits. Since the dielectric contrast between Si and a typical LC is not large, the crystal considered is taken to have the diamond structure due to its previous exceptional success in creating large PBGs in the low-lying bands of 3D PCs. In this work, we study the photonic band structure of the Si-based PC, and show the existence in this structure of a partial gap around X point. Specifically, it occurs between the 2nd and 3rd bands and, hence, in comparison with those in high-lying energy bands, is less receptive to imperfection

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in the system. Two forms of the structure are investigated, namely, (i) diamond-1 which is composed of LC spheres embedded in the Si background, and ii) diamond-2 (for contrast study) which is the inverse of diamond-1, with Si spheres immersed in the LC background. For each system, the study is carried out with the LC being in the isotropic (i.e., disordered)/nematic phase. We find a partial gap between the 2nd and 3rd bands, whose edge may be shifted by about 1% (in relative unit) when optical, thermal, or electrical means are applied to alter the phase of LC or rotate the axis of nematic molecules.

Our study employs a one-dimensional effective model, an improved version of conventional mean-field theory (MFT). A number of theoretical works in the category of MFT have been carried out to investigate the low-lying photonic states.^{19–22} The early MFT is focused on the long-wavelength limit, and replaces the PC under study by a mean medium with a single dielectric constant.^{19,20} In this limit, it simplifies greatly the analysis of light propagation in the PC, and offers the unique advantage of physical transparency, analytical capability, and computational efficiency. However, the approximation is only valid for the lowest states near $\mathbf{k}=0$ and, from a practical viewpoint, such a description is generally not sufficient, because, for PBG-based applications, it requires the knowledge of the bands around the PBG. We have developed an improved version of MFT (denoted as IMFT) in a series of work that extends the range of validity to the bands around the lowest PBG, while retaining partially the unique advantage of MFT. Preliminary results have been reported for 2D PCs.^{21,22} A full account of IMFT is presented in this work for 3D PCs.

The presentation is organized as follows. A detailed discussion is presented in Sec. II about the improved mean-field theory employed in our study. In Sec. III, we apply the theory to 3D Si-based PCs infiltrated with LC. A demonstrative example of FCC lattice composed of LC spheres embedded in the Si background is discussed, too, where we assess the validity of our mean-field method by comparing it with the plane wave expansion method. The FCC structure is also compared with diamond-1 and diamond-2, for the size of bandgap. Each diamond structure is examined with the LC being in the isotropic/nematic phase, and the partial gap around an X point is estimated for various orientations of nematic molecules as well as with LC being in the isotropic phase. Last, we summarize and conclude the study in Sec. IV.

II. THE 1D EFFECTIVE MODEL (IMFT)

In Sec. II A, we give a short introduction and a qualitative description of the theoretical model. In Sec. II B, we provide a full quantitative discussion of the theory.

A. Introduction

Various methods have been developed for the calculation of photonic band structure. For example, the plane wave method (PWM) is widely employed for its simplicity.^{9,11,23,24} The transfer matrix method is useful for calculating the transmission and reflection spectra which are directly measured in experiments.^{25–28} The finite difference time domain method is an important tool for investigating the property of cavity modes.²⁹ The Korringa–Kohn–Roster method

utilizes Green's function and calculates the density of states directly.³⁰ All of the foregoing methods are good for wide-frequency-range calculations and have been applied in search for useful structures of PCs. For many photonic devices, however, applications are based on the properties of just a few low-lying photonic bands. Mean-field-type theories such as the 1D effective model to be presented here are focused on the treatment of low-lying states and well-suited to such applications.

The core idea of the 1D model is sketched below. We consider a PC with a low-lying photonic state of wave vector $\mathbf{k}$. Let $|\mathbf{k}| \sim O(1/a)$ in the extended zone scheme, where a = lattice constant. In the conventional MFT, one would approximate the state by the single plane wave $|\mathbf{k}\rangle = e^{i\mathbf{k}\cdot\mathbf{r}}$. But the dielectric variation $\eta(\mathbf{r})$ in the direction of propagation [called longitudinal variation] results in Bragg scattering, which kicks the plane wave state $|\mathbf{k}\rangle = e^{i\mathbf{k}\cdot\mathbf{r}}$ into $|\mathbf{k}'\rangle = |\mathbf{k} + \mathbf{G}\rangle$ (with $\mathbf{G}/k$) and, in the case where $|\mathbf{k}'| \sim |\mathbf{k}|$, strongly mixes $|\mathbf{k}\rangle$ and $|\mathbf{k}'\rangle$. It thereby motivates us to treat $|\mathbf{k}\rangle$ and $|\mathbf{k}'\rangle$ on equal footing and resort to something like the multiplane wave expansion of fields which takes into account the strong mixing in discussion here, for $\mathbf{k}$ away from the neighborhood of $\mathbf{k}=0$. On the other hand, in the direction transverse to $\mathbf{k}$, since the field wavelength projected is infinite, we adopt the mean field approximation (valid in the long wavelength limit) or some variant form of it. In summary, (i) we average the transverse dielectric variation (perpendicular to the wave propagation) basically in accordance to the mean-field approximation, (ii) but account for the full details of longitudinal field/dielectric fluctuation (in the direction of wave propagation) via plane wave expansion of both the field/dielectric fluctuation. Extension is also made to incorporate the higher-order effect, namely, long-wavelength components of the transverse fluctuation. Such components may result in the kind of Bragg scattering, $|\mathbf{k}\rangle \rightarrow |\mathbf{k}'\rangle = |\mathbf{k} + \mathbf{G}\rangle$, with $\mathbf{G}$ not being in the longitudinal direction, and mix the plane waves.

B. Analytical capability

The improved mean field theory (IMFT) as proposed here is numerically more accurate than the conventional MFT, at the cost of raised level of complexity, though. As a result, the analytic capability of MFT is lost to a certain extent. However, as a 1D model, it is relatively simple and may thus still provide useful insights into the photonic band structure in 2D and 3D. A demonstrative example is given below before we plunge into a full quantitative account of IMFT. As shown in Fig. 1, we consider a 3D cubic PC formed from two dielectric materials, with the following dielectric variation in a unit cell (a = lattice constant)

$$\begin{aligned} \varepsilon(x, y, z) = \varepsilon_1, & \text{ for } (0 < x < x_c, 0 < y < x_c, 0 < z < x_c) \\ & \cup (0 < x < x_c, x_c < y < a, x_c < z < a) \\ & \cup (x_c < x < a, 0 < y < x_c, x_c < z < a) \\ & \cup (x_c < x < a, x_c < y < a, 0 < z < x_c), \\ \varepsilon(x, y, z) = \varepsilon_2, & \text{ otherwise,} \end{aligned}$$

which is a 3D version of the 2D checker board pattern. For a fixed lattice constant, let us ask how the size variation of the

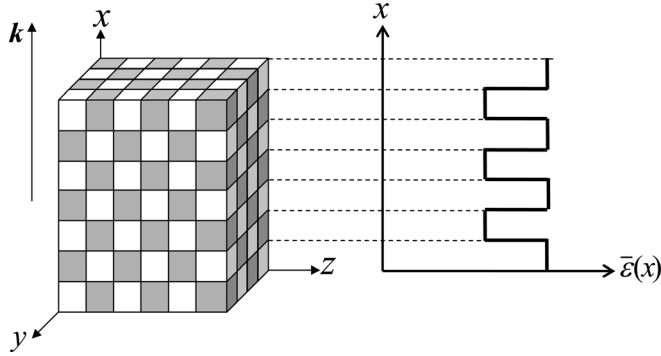


FIG. 1. An example of 3D PC illustrating the 1D effective model. The effective dielectric constant, $\bar{\epsilon}(x)$, is shown for the propagation in x direction.

1st gap depends on the composition ratio of the two dielectrics, a question which may well arise in applications. Now we employ the 1D effective model for analysis. Consider the direction of propagation along $(1, 0, 0)$. Then, a simple composition-weighted averaging of dielectric distribution, in the plane normal to the propagation, yields the following 1D effective dielectric variation along $(1, 0, 0)$,

$$\begin{aligned}\bar{\epsilon}(x) &= \frac{1}{a^2} \left\{ [x_c^2 + (a - x_c)^2] \epsilon_1 + 2x_c(a - x_c) \epsilon_2 \right\}, \\ &\quad \text{for } 0 < x < x_c, \\ &= \frac{1}{a^2} \left\{ [x_c^2 + (a - x_c)^2] \epsilon_2 + 2x_c(a - x_c) \epsilon_1 \right\}, \\ &\quad \text{for } x_c < x < a.\end{aligned}$$

This describes a Kronig–Penny-type lattice in the x direction and provides physical insight into the original 3D system. In particular, according to this 1D model, at $x_c = a/2$, $\bar{\epsilon}(x)$ becomes a constant, and the gap vanishes. Thus, for the propagation along $(1, 0, 0)$, the above analysis concludes that the gap is minimum with $x_c = a/2$ (corresponding to the 1:1 composition ratio). Our model greatly simplifies the analysis in this example, which is not possible with the conventional MFT or a numerical, full-range photonic band structure method.

C. Theory

Now, we begin the quantitative discussion of IMFT. Consider the propagation of a wave in a 3D PC. The H-field component of wave is governed by the Maxwell equation

$$\begin{aligned}-\nabla \times [\eta(\mathbf{r}) \nabla \times H(\mathbf{r})] &= \frac{\omega^2}{c^2} H(\mathbf{r}), \\ \nabla \cdot H(\mathbf{r}) &= 0.\end{aligned}\quad (1)$$

The field function satisfies the Bloch theorem, and can be expanded as

$$\begin{aligned}\mathbf{H}(\mathbf{r}) &= \sum_{\lambda, \mathbf{G}} \mathbf{H}_{\mathbf{G}}^{(\lambda)} e^{i(\mathbf{k} + \mathbf{G}) \cdot \mathbf{r}}, \\ (\mathbf{k} + \mathbf{G}) \cdot \mathbf{H}_{\mathbf{G}}^{(\lambda)} &= 0,\end{aligned}\quad (2)$$

where $\lambda = 1, 2$ denoting polarization, and $\mathbf{k}$ is the Bloch wave vector (in the extended zone scheme). The inverse dielectric distribution is similarly expanded

$$\eta(\mathbf{r}) \equiv \frac{1}{\epsilon(\mathbf{r})} = \sum_{\mathbf{G}} \eta_{\mathbf{G}} e^{i\mathbf{G} \cdot \mathbf{r}}. \quad (3)$$

The summation over $\mathbf{G}$ in each expansion runs through the reciprocal lattice of the PC. In order to solve Eq. (1), we separate the field/dielectric function both into longitudinal and transverse components, and perform mean-field type averaging of the transverse component, as discussed next.

D. Separation of longitudinal and transverse fluctuations

The task of separating longitudinal and transverse components is best done by introducing an auxiliary lattice. In order to distinguish between various lattices involved in the discussion, we call, throughout the presentation, the Bravais lattice of the PC in discussion lattice 1, the corresponding primitive cell, cell 1, and the reciprocal lattice, reciprocal lattice 1, while call the auxiliary lattice, lattice 2, the corresponding primitive cell, cell 2, and the reciprocal lattice reciprocal lattice 2.

First, for a given propagation direction, or wave vector $\mathbf{k}$, Appendix A shows that it is virtually always possible to choose a corresponding unit cell (which is not necessarily primitive) having the shape of a right parallelepiped with its axis aligned with $\mathbf{k}$, irrespective of the actual lattice and cell type. As shown in Fig. 2, the parallelepiped is spanned by the vectors $\{\mathbf{R}_{//}, \mathbf{R}_{\perp 1}, \mathbf{R}_{\perp 2}\}$, with $\mathbf{R}_{//}$ lying along $\mathbf{k}$ while $\mathbf{R}_{\perp 1}$ and $\mathbf{R}_{\perp 2}$ being transverse to $\mathbf{k}$ and spanning the base parallelogram of the parallelepiped. This parallelepiped constitutes cell 2, and the PC can alternatively be taken as the lattice (lattice 2) composed of cell 2's, with $\{\mathbf{R}_{//}, \mathbf{R}_{\perp 1}, \mathbf{R}_{\perp 2}\}$ being the corresponding primitive lattice vectors in this alternative description. We also introduce here the primitive lattice vectors $\{\mathbf{R}_1, \mathbf{R}_2, \mathbf{R}_3\}$ of lattice 1, and those of reciprocal lattice 1, $\{\mathbf{G}_1, \mathbf{G}_2, \mathbf{G}_3\}$, with $\mathbf{G}_k = (2\pi/|\mathbf{R}_1 \cdot \mathbf{R}_2 \times \mathbf{R}_3|) \sum_{ij} \epsilon_{ijk} \mathbf{R}_i \times \mathbf{R}_j$ (ϵ_{ijk} being the Levi-Civita symbol), as well as the primitive lattice vectors of reciprocal lattice 2, which are denoted as $\{\mathbf{G}_{//}^{(0)}, \mathbf{G}_{\perp 1}^{(0)}, \mathbf{G}_{\perp 2}^{(0)}\}$, with

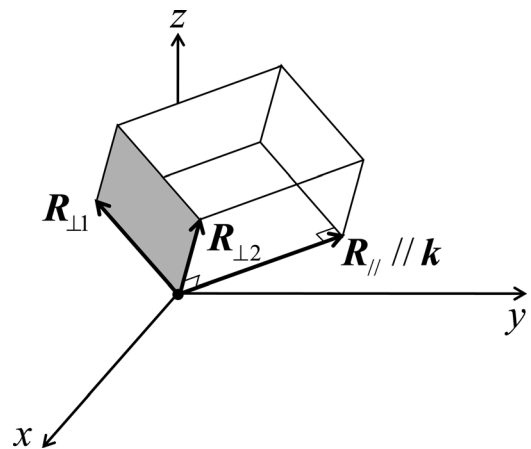


FIG. 2. The unit cell spanned by $\{\mathbf{R}_{//}, \mathbf{R}_{\perp 1}, \mathbf{R}_{\perp 2}\}$.

$$\begin{aligned}
\mathbf{G}_{//}^{(0)} &= 2\pi\mathbf{R}_{\perp 1} \times \mathbf{R}_{\perp 2} / [\mathbf{R}_{//} \cdot (\mathbf{R}_{\perp 1} \times \mathbf{R}_{\perp 2})], \\
\mathbf{G}_{\perp 1}^{(0)} &= 2\pi\mathbf{R}_{\perp 2} \times \mathbf{R}_{//} / [\mathbf{R}_{//} \cdot (\mathbf{R}_{\perp 1} \times \mathbf{R}_{\perp 2})], \\
\mathbf{G}_{\perp 2}^{(0)} &= 2\pi\mathbf{R}_{//} \times \mathbf{R}_{\perp 1} / [\mathbf{R}_{//} \cdot (\mathbf{R}_{\perp 1} \times \mathbf{R}_{\perp 2})], \\
\mathbf{G}_{//}^{(0)} // \mathbf{k}, \mathbf{G}_{\perp 1}^{(0)} \perp \mathbf{k}, \mathbf{G}_{\perp 2}^{(0)} \perp \mathbf{k}.
\end{aligned}$$

These vectors shall be used in the discussion

It is worthwhile to compare the two above descriptions of the same PC, namely, one in terms of {cell 1, lattice 1, reciprocal lattice 1} and the other in terms of {cell 2, lattice 2, reciprocal lattice 2}, and note a few useful facts. While {cell 1, lattice 1, reciprocal lattice 1} are the true primitive cell, lattice, and reciprocal lattice of the PC, {cell 2, lattice 2, reciprocal lattice 2} are the alternative description only introduced to facilitate the decomposition of transverse and longitudinal fluctuations. Generally speaking,

- (i) cell 2 is larger than the true primitive cell 1;
- (ii) lattice 2 is a subset of lattice 1; and
- (iii) reciprocal lattice 1 is a subset of reciprocal lattice 2.

It follows from (iii) that the set $\{e^{i\mathbf{G}\cdot\mathbf{r}}$, with $\mathbf{G} \in$ reciprocal lattice 2} contains spurious plane waves for the expansion of a periodic function defined on lattice 1. Similarly, according to (i) and (ii), we see that neither lattice 2 describes the true translational symmetry of the PC, nor cell 2 carries the true point symmetry of the system.

The auxiliary lattice provides an expedient vessel to the decomposition of transverse and longitudinal fluctuations, as follows. The inverse dielectric function $\eta(\mathbf{r})$ defined on lattice 1 can also be regarded as one defined on lattice 2. In particular, it is periodic both along $\mathbf{k}$, with $\eta(\mathbf{r}) = \eta(\mathbf{r} + \mathbf{R}_{//})$, and transverse to $\mathbf{k}$, with $\eta(\mathbf{r}) = \eta(\mathbf{r} + \mathbf{R}_{\perp 1}) = \eta(\mathbf{r} + \mathbf{R}_{\perp 2})$. The associated Fourier decomposition of $\eta(\mathbf{r})$ in these directions yields directly the separation of longitudinal and transverse components of dielectric fluctuation. A similar discussion applies to the field $\mathbf{H}(\mathbf{r})$.

Mathematically, the separation is carried out on each plane wave component, e.g., $e^{i\mathbf{G}\cdot\mathbf{r}}$ in the case of $\eta(\mathbf{r})$, or $e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}}$ in the case of $\mathbf{H}(\mathbf{r})$, where $\mathbf{G}$ belongs to reciprocal lattice 1. We decompose both $\mathbf{G}$ and $\mathbf{r}$ into longitudinal and transverse components, with $\mathbf{G} = \mathbf{G}_{//} + \mathbf{G}_{\perp}$ and $\mathbf{r} = \mathbf{r}_{//} + \mathbf{r}_{\perp}$. Then, the expansion $\mathbf{H}(\mathbf{r}) = \sum_{\lambda, \mathbf{G}} \mathbf{H}_{\mathbf{G}}^{(\lambda)} e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}}$ in Eq. (2) becomes

$$\begin{aligned}
\mathbf{H}(\mathbf{r}) &= \sum_{\mathbf{G}_{\perp}} \mathbf{H}_{\mathbf{G}_{\perp}}(r_{//}) e^{i\mathbf{G}_{\perp}\cdot\mathbf{r}_{\perp}}, \\
\mathbf{H}_{\mathbf{G}_{\perp}}(r_{//}) &\equiv e^{ikr_{//}} \sum_{\lambda, \mathbf{G}_{//}} \mathbf{H}_{\mathbf{G}_{\perp}, \mathbf{G}_{//}}^{(\lambda)} e^{i\mathbf{G}_{//}\cdot\mathbf{r}_{//}}, \\
[(k + G_{//})\hat{\mathbf{k}} + \mathbf{G}_{\perp}] \cdot \mathbf{H}_{\mathbf{G}_{\perp}, \mathbf{G}_{//}}^{(\lambda)} &= 0.
\end{aligned} \quad (4)$$

Here, $\hat{\mathbf{k}} \equiv \mathbf{k}/|\mathbf{k}|$. Eq. (4) expands $\mathbf{H}(\mathbf{r})$ as a sum of $\{e^{i\mathbf{G}_{\perp}\cdot\mathbf{r}_{\perp}}\}$ which are transverse fluctuations, and $\mathbf{H}_{\mathbf{G}_{\perp}}(r_{//})$ as a sum of $\{e^{i(k+G_{//})r_{//}}\}$ which are longitudinal fluctuations. If we keep only the $\mathbf{G}_{\perp} = 0$ term in the expansion of $\mathbf{H}(\mathbf{r})$, then $\mathbf{H}(\mathbf{r}) \approx \mathbf{H}_{\mathbf{G}_{\perp}=0}(r_{//})$ showing vanishing $\mathbf{r}_{\perp}$ dependence. This is the lowest-order approximation of our model where the transverse fluctuation is entirely neglected. However, even at this level of approximation, we have

$$\mathbf{H}(\mathbf{r}) \approx \mathbf{H}_{\mathbf{G}_{\perp}=0}(r_{//}) = \sum_{\lambda, \mathbf{G}_{//}} \mathbf{H}_{\mathbf{G}_{\perp}, \mathbf{G}_{//}}^{(\lambda)} e^{i(k+G_{//})r_{//}} |_{\mathbf{G}_{\perp}=0},$$

and it still accounts fully for the $\mathbf{r}_{\perp}$ dependence or longitudinal fluctuation. This is why our model is regarded as an improvement over the conventional MFT. Further refinement of the model can be made by the retention in Eq. (4) of a few long-wavelength components of transverse fluctuation (with $\mathbf{G}_{\perp} \neq 0$), e.g.,

$$\mathbf{H}(\mathbf{r}) \approx \sum_{\mathbf{G}_{\perp} \leq |\mathbf{G}_c(\mathbf{k})|} \mathbf{H}_{\mathbf{G}_{\perp}}(r_{//}) e^{i\mathbf{G}_{\perp}\cdot\mathbf{r}_{\perp}},$$

where $G_c(\mathbf{k})$ is a pre-chosen $\mathbf{k}$ -dependent cutoff of $\mathbf{G}_{\perp}$. We note that the refinement takes care of the plane wave mixing due to the kind of Bragg scattering, $|\mathbf{k}\rangle \rightarrow |\mathbf{k}'\rangle = |\mathbf{k} + \mathbf{G}_{\perp} + \mathbf{G}_{//}\rangle$ (with $|\mathbf{G}_{\perp}| \leq G_c(\mathbf{k})$).

Equation (4) expands the $\mathbf{H}$ -field in terms of plane waves $e^{i\mathbf{G}_{\perp}\cdot\mathbf{r}_{\perp}}$'s and $e^{i(k+G_{//})r_{//}}$'s. The wave vectors $\mathbf{G}_{//}$ and $\mathbf{G}_{\perp}$ here (which are the projections of $\mathbf{G}$ onto $\mathbf{k}$ and transverse to $\mathbf{k}$, respectively) actually belong to reciprocal lattice 2. We write $\mathbf{G}_{//} = n_{//}\mathbf{G}_{//}^{(0)}$ and $\mathbf{G}_{\perp} = n_{\perp 1}\mathbf{G}_{\perp 1}^{(0)} + n_{\perp 2}\mathbf{G}_{\perp 2}^{(0)}$, and reexpress Eq. (4)

$$\begin{aligned}
\mathbf{H}(\mathbf{r}) &= \sum_{n_{\perp 1}, n_{\perp 2}} \mathbf{H}_{\mathbf{G}_{\perp}}(r_{//}) e^{i(n_{\perp 1}\mathbf{G}_{\perp 1}^{(0)} + n_{\perp 2}\mathbf{G}_{\perp 2}^{(0)})\cdot\mathbf{r}_{\perp}}, \\
\mathbf{H}_{\mathbf{G}_{\perp}}(r_{//}) &\equiv e^{ikr_{//}} \sum_{\lambda, n_{//}} \mathbf{H}_{\mathbf{G}_{\perp}, n_{//}}^{(\lambda)} e^{in_{//}\mathbf{G}_{//}^{(0)}\cdot\mathbf{r}_{//}}.
\end{aligned} \quad (4')$$

Notably, reciprocal lattice 1 used in Eq. (2) has been replaced by reciprocal lattice 2 in Eq. (4'), and caution must be exercised in interpreting the equation since *reciprocal lattice 1* $\subset$ *reciprocal lattice 2* as mentioned earlier. Spurious terms are expected to appear in Eq. (4') and must be removed. Appendix B derives the constraint on $n_{//}$, $n_{\perp 1}$, and $n_{\perp 2}$ which removes the spurious terms. Note that Eq. (4') also provides an explicit way to determine the plane wave cut-off used in the expansion of longitudinal and transverse fluctuations. For example, one can set $n_{\perp 1} \leq n_{\perp 1}^{(c)}$, $n_{\perp 2} \leq n_{\perp 2}^{(c)}$ for the expansion of transverse fluctuation, with the parameter $n_{\perp i}^{(c)}$, $i = 1, 2$ being determined by the cutoff $G_c(\mathbf{k})$ via the equation $G_c(\mathbf{k}) = n_{\perp i}^{(0)} |\mathbf{G}_{\perp i}^{(0)}|$.

The inverse dielectric constant can be decomposed similarly as

$$\begin{aligned}
\eta(\mathbf{r}) &= \sum_{\mathbf{G}_{\perp}} \eta_{\mathbf{G}_{\perp}}(r_{//}) e^{i\mathbf{G}_{\perp}\cdot\mathbf{r}_{\perp}}, \\
\eta_{\mathbf{G}_{\perp}}(r_{//}) &\equiv \sum_{\mathbf{G}_{//}} \eta_{\mathbf{G}_{\perp}, \mathbf{G}_{//}} e^{i\mathbf{G}_{//}\cdot\mathbf{r}_{//}},
\end{aligned} \quad (5)$$

with $\mathbf{G}_{//}$ and $\mathbf{G}_{\perp}$ subject to the same constraint derived in Appendix B.

Substituting the expansions (4') and (5) into the Maxwell Eq. (1), we obtain the equation for the longitudinal fluctuation $\mathbf{H}_{\mathbf{G}_{\perp}}(r_{//})$,

$$\begin{aligned}
& - \sum_{\mathbf{G}'_{\perp}} (\hat{\mathbf{R}}_{//} \partial_{//} + \mathbf{G}_{\perp}) \times \eta_{\mathbf{G}_{\perp} - \mathbf{G}'_{\perp}}(r_{//}) \left[(\hat{\mathbf{R}}_{//} \partial_{//} + \mathbf{G}'_{\perp}) \times \mathbf{H}_{\mathbf{G}'_{\perp}}(r_{//}) \right] \\
& = \frac{\omega^2}{c^2} \mathbf{H}_{\mathbf{G}_{\perp}}(r_{//}), \quad |\mathbf{G}_{\perp}| \leq G_c(k),
\end{aligned} \quad (6)$$

where $\hat{\mathbf{R}}_{//} \equiv \mathbf{R}_{//}/|\mathbf{R}_{//}|$. Eq. (6) is the central equation in our theory. $\mathbf{H}_{\mathbf{G}_{\perp}}(r_{//})$'s at various $\mathbf{G}_{\perp}$'s are coupled and Eq. (6) provides the set of coupled equations. The coupled equations can be solved with PWM, by expanding each $\mathbf{H}_{\mathbf{G}_{\perp}}(r_{//})$ [as in Eq. (4')] and each $\eta_{\mathbf{G}_{\perp}}(r_{//})$ [as in Eq. (5)]. In the lowest-order approximation, the transverse fluctuation is completely neglected, and only the $\mathbf{G}_{\perp} = 0$ term is kept in the expansion of H and η . Eq. (6) then reduces to the single equation

$$-\partial_{//}\eta_{\mathbf{G}_{\perp}=0}(r_{//})\partial_{//}\mathbf{H}_{\mathbf{G}_{\perp}=0}(r_{//}) = \frac{\omega_0^2}{c^2}\mathbf{H}_{\mathbf{G}_{\perp}=0}(r_{//}). \quad (7)$$

This represents the wave equation in 1D with the inverse dielectric distribution being $\eta_{\mathbf{G}_{\perp}=0}(r_{//})$.

Equation (6) is also applicable to the 2D PCs with dielectric columns. If we define the z direction to be along the columns, then for TE modes, $\mathbf{H}/\hat{z}$ ($\hat{z}$ = unit vector in the z direction). Moreover, $\partial_z \varepsilon(\mathbf{r}) = \partial_z \mathbf{H}(\mathbf{r}) = \partial_z \mathbf{E}(\mathbf{r}) = 0$, and $\mathbf{k}$ is always restricted to be in the x - y plane. For TE modes, Eq. (6) is reduced to

$$\begin{aligned} & -\sum_{\mathbf{G}'_{\perp}} \left(\partial_{//}\eta_{\mathbf{G}_{\perp}-\mathbf{G}'_{\perp}}(r_{//})\partial_{//} + \eta_{\mathbf{G}_{\perp}-\mathbf{G}'_{\perp}}(r_{//})\mathbf{G}_{\perp}\mathbf{G}'_{\perp} \right) \mathbf{H}_{\mathbf{G}'_{\perp}}(r_{//}) \\ & = \frac{\omega^2}{c^2}\mathbf{H}_{\mathbf{G}_{\perp}}(r_{//}). \end{aligned}$$

For TM modes, on the other hand, we have $\mathbf{E}/\hat{z}$ ($\mathbf{E}$ = the electric field). In this case, the wave equation of E -field [analogous to Eq. (1)] is utilized, leading to an equation for the various components $\mathbf{E}_{\mathbf{G}_{\perp}}(r_{//})$'s, which is similar to the last equation:

$$-\sum_{\mathbf{G}'_{\perp}} \eta_{\mathbf{G}_{\perp}-\mathbf{G}'_{\perp}}(r_{//}) \left(\partial_{//}^2 + (\mathbf{G}'_{\perp})^2 \right) \mathbf{E}_{\mathbf{G}'_{\perp}}(r_{//}) = \frac{\omega^2}{c^2}\mathbf{E}_{\mathbf{G}_{\perp}}(r_{//}).$$

Both equations have been derived previously.^{21,22}

E. Degenerate perturbation theory for states near the B.Z. boundary

In principle, if one sets the transverse fluctuation cutoff $G_c(\mathbf{k}) = \infty$, then Eq. (6) includes all Bragg coupling among plane waves and, therefore, is equivalent to the conventional PWM. However, as we mentioned earlier, our 1D model approximates Eq. (6) by retaining only a few components of transverse fluctuation [selected with the condition $|\mathbf{G}_{\perp}| \leq G_c(k)$] in the calculation. Such a cutoff of transverse fluctuation is reasonable in most cases, but may lose some important Bragg coupling for the states near Brillouin zone (B.Z.) boundary, if the PC owns nontrivial point symmetry. Degenerate perturbation theory is discussed below to solve this problem for the states near B.Z. boundary.

First, we explain how the problem arises. Consider the case where $\mathbf{k}$ lies right on B.Z. boundary, and choose, for the sake of simplicity, the cutoff $G_c(\mathbf{k}) = 0$. Let $\hat{R}$ be a symmetry operator ($\in$ the point symmetry group) to which there corresponds the Bragg scattering $|\mathbf{k}\rangle \rightarrow |\mathbf{k}'\rangle = \hat{R}|\mathbf{k}\rangle = |\mathbf{k} + \mathbf{G}\rangle$ with $|\mathbf{k}| = |\mathbf{k}'|$. In the case where $\mathbf{k}$ is a point of high symmetry, the scattering may occur with $\mathbf{G}/\mathbf{k}$. (For example,

in the case of a cubic PC, $|\mathbf{k}_x\rangle \rightarrow |-\mathbf{k}_x\rangle$ with $\mathbf{G} = -2\mathbf{k}_x$, where $\mathbf{k}_x$ = X-point wave vector.) In such a case, the scattering is derived from the longitudinal dielectric fluctuation which is already included in the 1D model. However, in the general case, $\mathbf{k}$ is not a high symmetry point. Therefore, the vector $\mathbf{G}$ above may not be parallel to $\mathbf{k}$ or, in other words, the projection $\mathbf{G}_{\perp} \neq 0$. The strong mixing between $|\mathbf{k}\rangle$ and $|\mathbf{k}' = \mathbf{k} + \mathbf{G}_{\perp} + \mathbf{G}_{//}\rangle$ is then inappropriately excluded from the calculation since $|\mathbf{G}_{\perp}|_c(\mathbf{k})$ [with $G_c(\mathbf{k}) = 0$ here]. Therefore, a further improvement which incorporates the mixing is required for the model. In the following, we consider the case of a finite $G_c(\mathbf{k})$, and discuss the improvement.

Generally, the coupling missed in Eq. (6) between plane waves corresponds to the kind of Bragg scattering, $|\mathbf{k}\rangle \rightarrow |\mathbf{k}_i = \mathbf{k} + \mathbf{G}^{(i)}\rangle$, $i = 1, 2, \dots, n$, with $|\mathbf{k}| \sim |\mathbf{k}_i|$ and $|\mathbf{G}^{(i)}| > G_c(\mathbf{k})$ (where $\mathbf{G}^{(i)}$ is the transverse projection of $\mathbf{G}^{(i)}$). Since $|\mathbf{k}| \sim |\mathbf{k}_1| \sim |\mathbf{k}_2| \dots$ and so on, the degenerate perturbation theory can be applied to treat the coupled plane waves $|\mathbf{k}_i\rangle$'s, $i = 0, 1, 2, \dots, n$, (with $\mathbf{k}_{i=0} \equiv \mathbf{k}$) all on equal footing. Moreover, we also include, for each $|\mathbf{k}_i\rangle$, $|\mathbf{k}_i + \mathbf{G}_{\perp} + \mathbf{G}_{//}\rangle$'s which are coupled to $|\mathbf{k}_i\rangle$ [subject to the condition $|\mathbf{G}_{\perp}(\mathbf{k}_i)| < G_c(\mathbf{k}_i)$]. Altogether, in order to improve the calculation of the state at $\mathbf{k}$, we expand the set of plane waves, from the original set $\{|\mathbf{G}_{//}(\mathbf{k}) + \mathbf{G}_{\perp}(\mathbf{k})\rangle$'s, $|\mathbf{G}_{\perp}(\mathbf{k})| < G_c(\mathbf{k})\}$ to the union $\cup_{i=0,1,\dots,n} \{|\mathbf{G}_{//}(\mathbf{k}_i) + \mathbf{G}_{\perp}(\mathbf{k}_i)\rangle$'s, $|\mathbf{G}_{\perp}(\mathbf{k}_i)| < G_c(\mathbf{k}_i)\}$. (The forgoing expressions are written with the dependence of $\mathbf{G}_{//}$ and $\mathbf{G}_{\perp}$ on $\mathbf{k}_i$ being stressed.) In the next section, numerical calculations will be presented based on the above method.

F. Computational efficiency

We compare the improved mean-field theory with the ordinary plane wave method, and make a short remark on the computational efficiency. For 3D PCs, the number of plane waves $\{e^{i\mathbf{G}\cdot\mathbf{r}}\}$ used in PWM is approximately N^3 , where N = the number of plane waves with $\mathbf{G}$'s in a given direction determined by the wave vector cutoff in PWM. The size of the matrix constructed for the eigenvalue Eq. (1) is $N^3 \times N^3$. In our case, we need approximately $p \times p \times N'$, where p/N' = the number of plane waves in a given transverse/the longitudinal direction (with respect to the wave vector $\mathbf{k}$) determined by the corresponding cutoff. The size of the matrix constructed for the eigenvalue Eq. (1) is $p^2 N' \times p^2 N'$. In a typical case, $p < N$ and $N' \sim N$. Therefore, from the computational viewpoint, IMFT uses less memory space, as well as saves CPU time for matrix diagonalization (in solving the eigenvalue equation).

We remark on the accuracy of IMFT. The present IMFT successfully marries the conventional MFT and the PWM, providing a systematic way to move from the extreme of the conventional MFT (where the whole structure is replaced by a mean uniform medium) to the extreme of the PWM (where the details of dielectric fluctuation are all accounted for). The number of plane waves included in the calculation may vary from one (e.g., $e^{i\mathbf{k}\cdot\mathbf{r}}$ in the conventional MFT) to hundreds or thousands (in the PWM), as determined by the transverse cutoff parameter, $G_c(\mathbf{k})$. For the calculation of low-lying bands, the IMFT is efficient and accurate. For

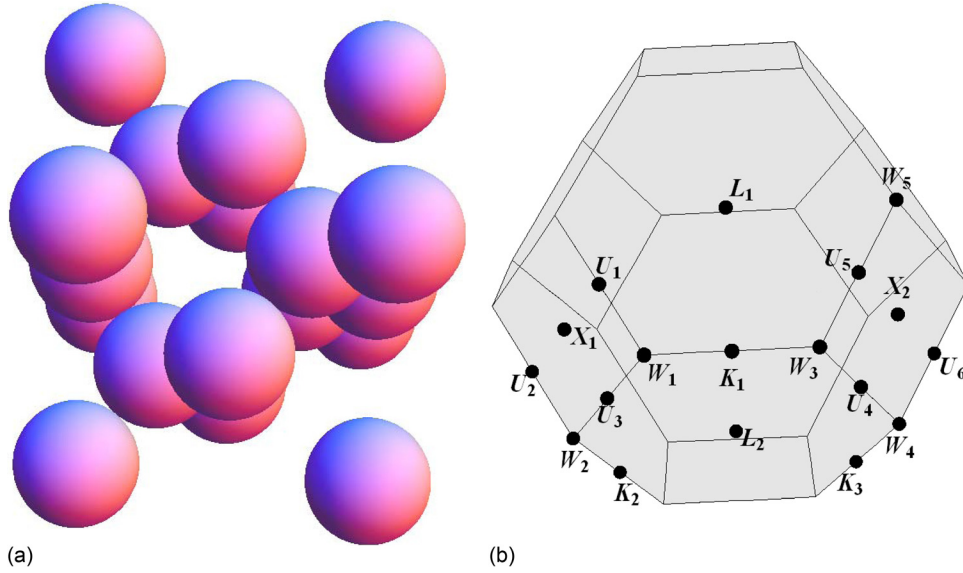


FIG. 3. (Color online) (a) Si/LC spheres stacked to form diamond-1/diamond-2. (b) The Brillouin zone of FCC lattice, with the symmetry points $L_1: \frac{2\pi}{a}(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$, $L_2: \frac{2\pi}{a}(\frac{1}{2}, \frac{1}{2}, -\frac{1}{2})$, $K_1: \frac{2\pi}{a}(\frac{3}{4}, \frac{3}{4}, 0)$, $K_2: \frac{2\pi}{a}(\frac{3}{4}, 0, \frac{3}{4})$, $K_3: \frac{2\pi}{a}(0, \frac{3}{4}, \frac{3}{4})$, $X_1: \frac{2\pi}{a}(1, 0, 0)$, $X_2: \frac{2\pi}{a}(0, 1, 0)$, $W_1: \frac{2\pi}{a}(1, \frac{1}{2}, 0)$, $W_2: \frac{2\pi}{a}(1, 0, \frac{1}{2})$, $W_3: \frac{2\pi}{a}(\frac{1}{2}, 1, 0)$, $W_4: \frac{2\pi}{a}(0, 1, \frac{1}{2})$, $W_5: \frac{2\pi}{a}(\frac{1}{2}, \frac{1}{2}, 1)$, $U_1: \frac{2\pi}{a}(1, \frac{1}{4}, \frac{1}{4})$, $U_2: \frac{2\pi}{a}(1, \frac{1}{4}, -\frac{1}{4})$, $U_3: \frac{2\pi}{a}(1, -\frac{1}{4}, \frac{1}{4})$, $U_4: \frac{2\pi}{a}(\frac{1}{4}, 1, \frac{1}{4})$, $U_5: \frac{2\pi}{a}(\frac{1}{4}, 1, -\frac{1}{4})$, and $U_6: \frac{2\pi}{a}(-\frac{1}{4}, 0, \frac{1}{4})$.

high-lying bands or structures with highly contrasting dielectric constants, the IMFT employs a plane wave set virtually the same as that in the PWM. In this case, the accuracy in the two methods (IMFT and PWM) is basically the same.

III. 3D PCS INFILTRATED WITH LC

In this section, IMFT is employed to calculate the band structures of 3D PCs. Firstly, we compare IMFT with PWM for an assessment of IMFT. This is carried out with the system of a closely packed FCC composed of LC spheres embedded in Si background. Then, we present the band structures of diamond-1 and diamond-2. Throughout the work, we take the refractive index $n = 3.464$ for Si. For liquid crystal, we choose LC 5CB as an example. We take the refractive indices $n_e = 1.706$ (in the extraordinary direction), $n_o = 1.522$ (in the ordinary direction), and $n = 1.586$ (in the isotropic phase).³¹

Figure 3 shows the diamond crystal structure, and the corresponding Brillouin zone of FCC along with various symmetry points, which shall be used in the presentation of band structures.

In Fig. 4, the band structure of the FCC is plotted, which is calculated with both PWM and IMFT for comparison. LC is taken to be in the nematic phase, and the axis of nematic molecules is placed along the (1,1,1) direction. Firstly, the number of plane waves used in PWM is 4913 ($= 17^3$), while that used in IMFT varies with the direction of wave propagation, from 935 to 2021. Although IMFT uses less plane waves, the result agrees reasonably well with that calculated by PWM. Secondly, the low-lying bands here do not show either any full gap, or even any partial gap over a sizable portion of B.Z. This result is suggestive and directs our search/study to the diamond structure discussed next.

Two systems are investigated. Diamond-1 is composed of identical LC spheres in touch with one another and stacked to form a diamond structure, with the structure embedded in the Si background. For contrast study, we also consider another diamond structure, namely, diamond-2.

Diamond-2 is the inverse structure of diamond-1, with Si and LC interchanged, where LC is infiltrated into the void between spheres. For practical purpose, the spheres may be approximated and replaced by wheels so that the structure can be fabricated with the layer-by-layer lithography of Si technology. This is shown in Fig. 5 for a proposed (1, 1, 1)-grown system and Fig. 6 for a (1, 0, 0)-grown system. Note that the wheels are connected by rods, in order to form percolating channels facilitating the infiltration of LC, in the case of diamond-1, or form the backbone in the case of diamond-2. We expect that the deviation from exact spherical geometry (in using wheels here) should not affect qualitatively the discussion below, which is focused on the low-lying bandgap of diamond-1/diamond-2 composed of spheres. It is known that the low-lying gap in the diamond structure is robust against geometric deviation to some extent, as shown in the previous work where a rod-hole structure was proposed in place of the exact diamond structure for fabrication.¹⁰

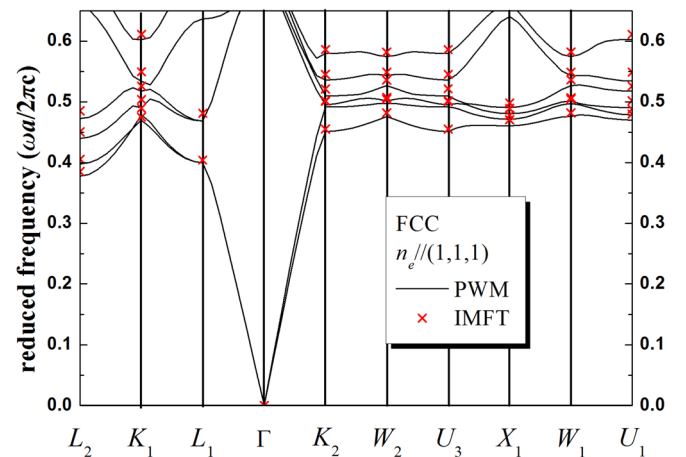


FIG. 4. (Color online) Comparison between PWM and IMFT in the case of a closely packed FCC lattice composed of 5CB spheres embedded in the Si background. Solid lines – PWM, “x” – IMFT. The number of plane waves used in IMFT varies, from 935 to 2021, for propagation along different symmetry directions, while PWM uses 4913 plane waves.

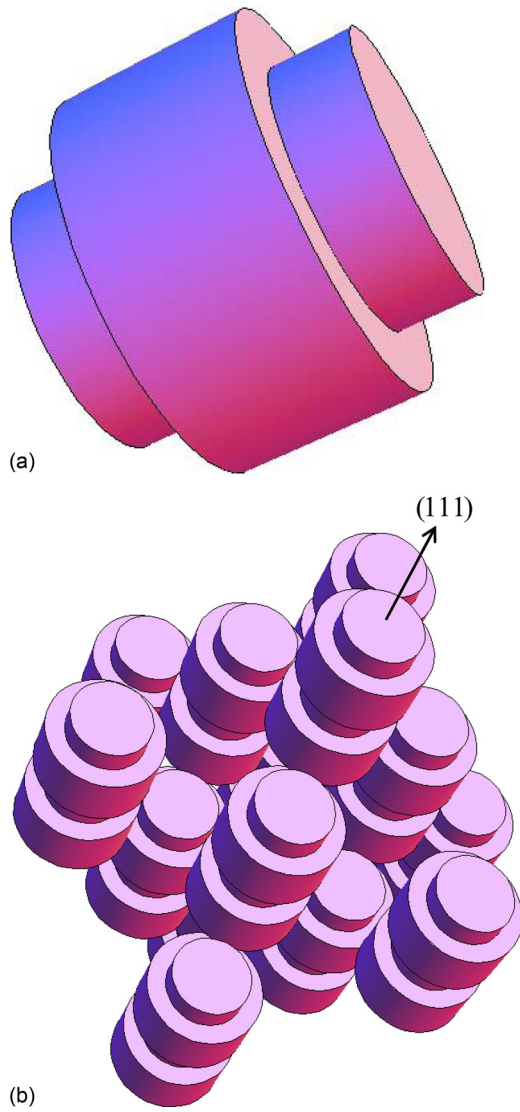


FIG. 5. (Color online) Diamond-1/diamond-2 may be grown in (1 1 1) direction with Si technology. (a) The building block that approximates the sphere of Si/LC has the shape of a wheel. (b) Wheels are stacked to form a diamond structure.

For each diamond system, the following cases are considered according to the state of LC, which can be (a) nematic phase, with the LC director $\hat{n}_e/(1, 1, 1)$; (b) nematic phase, with $\hat{n}_e/(1, 0, 0)$; (c) nematic phase, with $\hat{n}_e/(0, 1, 1)$; and (d) isotropic phase.

Figure 7 presents the band structure of diamond-1 in the four cases. As shown in the graph, a partial gap denoted as $PG(X)$ is well defined in a fraction ($\sim$ a few tenths) of B.Z., which is indicated by the gray stripe and centered around X_2 -point (located in the (0, 1, 0) direction). The gap-to-midgap ratio is

- 3.8% for $\hat{n}_e/(1, 1, 1)$ [in Fig. 7(a)],
- 4.5% for $\hat{n}_e/(1, 0, 0)$ [in Fig. 7(b)],
- 5.5% for $\hat{n}_e/(0, 1, 1)$ [in Fig. 7(c)], and
- 5.3% with isotropic LC [in Fig. 7(d)].

The partial gap itself can be used to filter light incident approximately in a special direction (i.e., within a reasonable

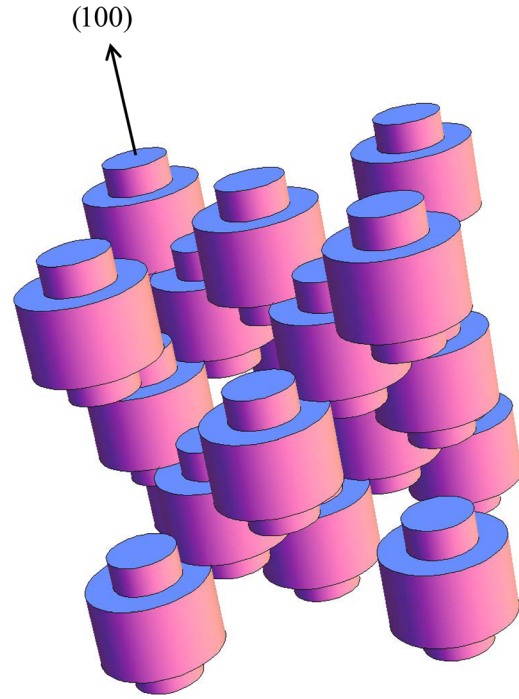


FIG. 6. (Color online) Diamond-1/diamond-2 may also be grown in (1 0 0) direction with Si technology.

range of solid angle around the direction),¹¹ e.g., (0, 1, 0) in our case.

Moreover, Fig. 7 shows that the upper edge of $PG(X)$ [denoted as $PG^+(X)$] is located at X_2 , and shifts with the orientation of $\hat{n}_e$ or phase transition of LC. We have (in units of $\omega a/2\pi c$)

- $PG^+(X) \sim 0.3661$ for $\hat{n}_e/(1, 1, 1)$ [in Fig. 7(a)],
- $PG^+(X) \sim 0.3680$ for $\hat{n}_e/(0, 0, 1)$ [in Fig. 7(b)],
- $PG^+(X) \sim 0.3715$ for $\hat{n}_e/(1, 1, 0)$ [in Fig. 7(c)], and
- $PG^+(X) \sim 0.3704$ for isotropic LC [in Fig. 7(d)]

The relative shift in $PG^+(X)$ is listed in the following for potential applications,

- (i) $\delta[PG^+(X)]/PG^+(X) \sim 0.96\%$, when the LC is in the nematic phase with $\hat{n}_e$ being switched between (1, 1, 0) and (0, 0, 1);
- (ii) $\delta[PG^+(X)]/PG^+(X) \sim 0.66\%$, when the LC is switched between the nematic phase [with $\hat{n}_e/(0, 0, 1)$] and the isotropic phase.

The magnitude of the relative shift derived here is comparable to that reported for 1D Si-based PCs infiltrated with LC.¹⁸ Moreover, the shift in $PG^+(X)$ may be utilized to provide the function of filtering, modulating, or on-off switching, for the light with a frequency close to $PG^+(X)$. This can be achieved through electrical, optical, or thermal tuning, as follows. Based on the result in (i), a configuration is depicted in the inset of Fig. 7(c) suitable for electrical tuning. The PC is (1, 0, 0) grown, and the light is incident in the (0, 1, 0) direction (in the plane). The LC molecule is rotated by electric fields applied in the (0, 1, 1) (in the plane) or (1, 0, 0) (normal to the plane) directions. On the other hand,

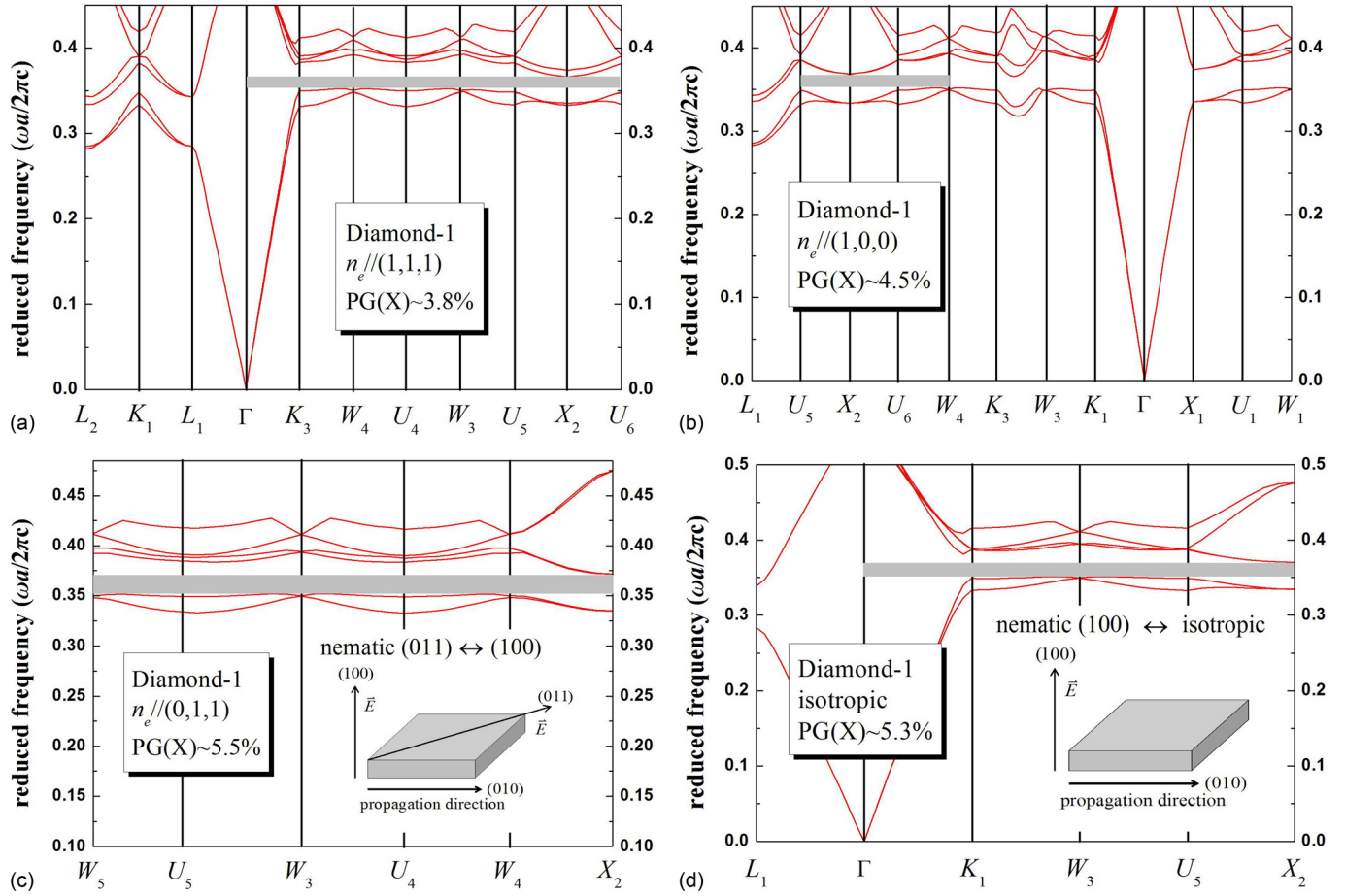


FIG. 7. (Color online) Band structures of diamond-1 for various LC director $\hat{n}_e$. (a) $\hat{n}_e // (1, 1, 1)$; (b) $\hat{n}_e // (1, 0, 0)$; (c) $\hat{n}_e // (0, 1, 1)$; (d) LC in isotropic phase. The inset of (c) shows the configuration for electrical tuning. The inset of (d) shows the configuration for electrical/thermal/optical tuning.

according to the result in (ii), thermal or optical tuning is also possible, in the configuration depicted in the inset of Fig. 7(d). The configuration is basically the same as the previous one, except for the absence of electric field in the (0, 1, 1) direction. The electric field is applied only in the (1, 0, 0) to orient the LC molecule in the nematic phase. Thermal or optical methods are used to induce the required nematic $\leftrightarrow$ isotropic phase transition of LC. Last, in relation to the application envisioned here, we note that on-off switching in the sub-THz range has been demonstrated for 2D PCs infiltrated with LC 5CB.¹⁷

Figure 8 presents the band structure of diamond-2. As shown in the graph, a partial gap around X_2 -point is also well defined. The gap-to-midgap ratio is

- 5.2% for $\hat{n}_e // (1, 1, 1)$ [in Fig. 8(a)],
- 7.4% for $\hat{n}_e // (1, 0, 0)$ [in Fig. 8(b)],
- 8.9% for $\hat{n}_e // (0, 1, 1)$ [in Fig. 8(c)], and
- 8.7% with isotropic LC [in Fig. 8(d)]

For the upper edge of $PG(X)$, we have (in units of $\omega/2\pi c$)

- $PG^+(X) \sim 0.4754$ for $\hat{n}_e // (1, 1, 1)$ [in Fig. 8(a)],
- $PG^+(X) \sim 0.4820$ for $\hat{n}_e // (1, 0, 0)$ [in Fig. 8(b)],
- $PG^+(X) \sim 0.4903$ for $\hat{n}_e // (0, 1, 1)$ [in Fig. 8(c)], and
- $PG^+(X) \sim 0.4871$ for isotropic LC [in Fig. 8(d)]

The relative shift in $PG^+(X)$ is listed in the following,

- $\delta[PG^+(X)]/PG^+(X) \sim 1.7\%$, when $\hat{n}_e$ is switched between (0, 1, 1) and (1, 0, 0);
- $\delta[PG^+(X)]/PG^+(X) \sim 1\%$, when LC is switched between the nematic phase [with $\hat{n}_e // (1, 0, 0)$] and the isotropic phase.

It shows a generally larger degree of tuning with diamond-2 than with diamond-1. This is a reasonable result. Since the tuning derives from the birefringent property of LC, it increases with the compositional fraction of LC, and thus diamond-2 prevails over diamond-1 as can be easily deduced.

We make a few remarks on the fabrication procedure for the structure of diamond-1, shown in Fig. 6. The layer-by-layer procedure includes material deposition, aligned lithography, etching, and planarization in one cycle, which has already been successfully employed in the growth of rod-hole structures.³² Because building elements in our case consist of cylinders with various radii, as opposed to only one radius in the rod-hole structure, the procedure has to be extended. After a few cycles, the material inside the percolating network of cylinders can be removed by wet etching,³² leaving voids and Si skeleton. The voids can be filled by LC, at the last step of growth.

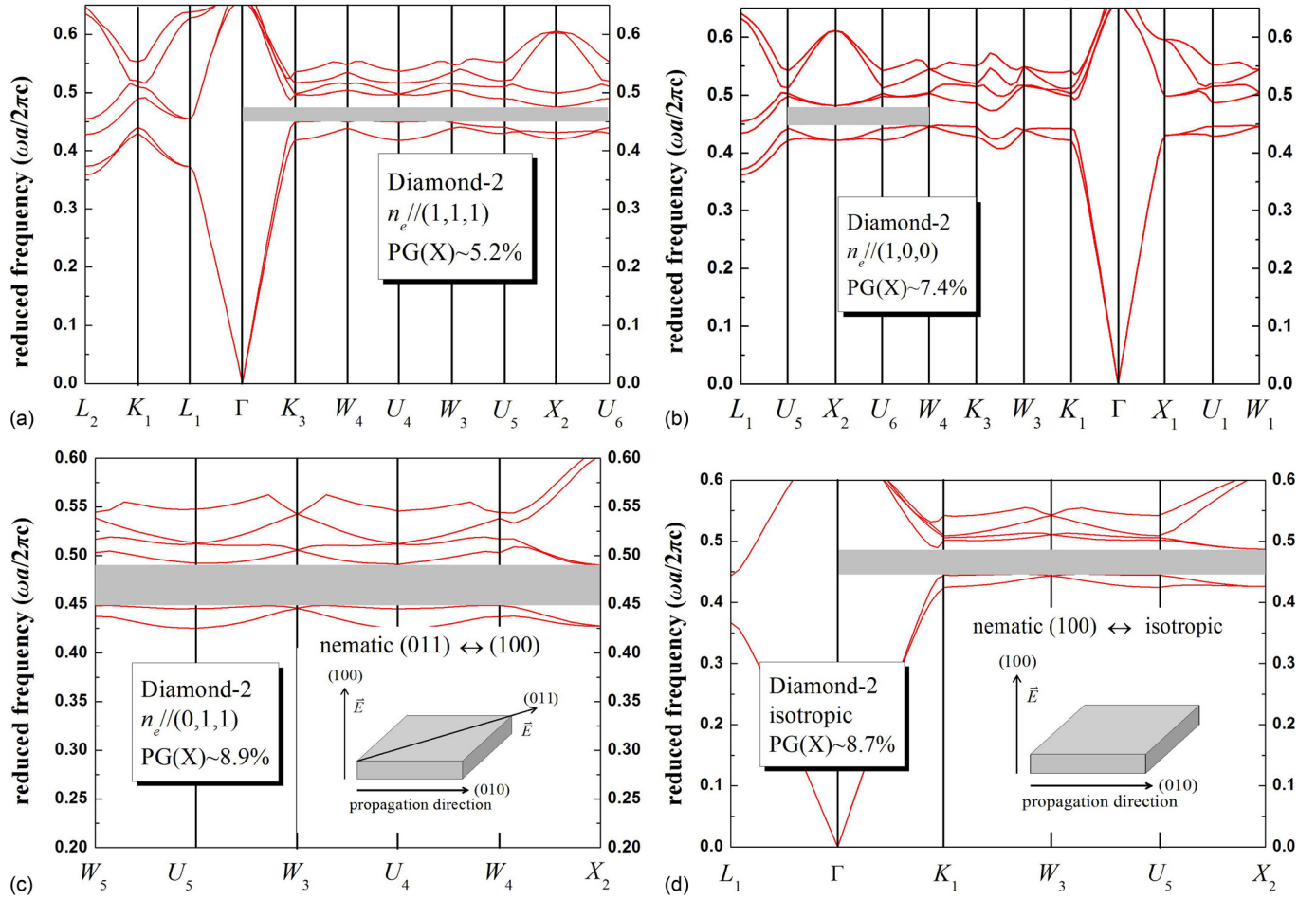


FIG. 8. (Color online) Band structures of diamond-2 for various LC director $\hat{n}_e$. (a) $\hat{n}_e // (1,1,1)$ (b) $\hat{n}_e // (1,0,0)$ (c) $\hat{n}_e // (0,1,1)$; (d) LC in the isotropic phase. The inset of (c) shows the configuration for electrical tuning. The inset of (d) shows the configuration for electrical/thermal/optical tuning.

IV. CONCLUSION

An improved version (IMFT) of mean-field theory has been presented and successfully applied to 3D PCs of FCC or diamond structures. IMFT is basically a 1D effective model of 3D systems, which describes fully the dielectric variation in the direction of wave propagation, but takes mean field average in the transverse direction. While retaining partially the advantage of mean field theory, it improves in numerical accuracy and extends the MFT range of validity to low-lying bands. The theory has been employed to investigate Si-based PCs infiltrated with LC, with the LC being in the isotropic/nematic phase. Overall, the diamond structure shows the existence of a low-lying partial gap, which has a reasonable size (with gap-to-midgap ratio $\sim$ a few percent) over a fraction ($\sim$ a few tenths) of B.Z., but the FCC structure does not. The partial gap occurs around an X point, and is estimated for various orientations of nematic molecules or with the LC being in the isotropic phase. It can be tuned by electrical, thermal, or optical means, and examples of configurations suitable for the tuning have been examined with a $(0,0,1)$ -grown diamond structure. The magnitude of gap edge tunability in these configurations is found to be $\sim 1\%$. Finally, the structure of PCs envisioned here is compatible with the layer-by-layer fabrication of semiconductor technology, and thus may be useful for the application of photonic

integrated circuits. In order to optimize the performance of the PC considered here in the aspect of gap tunability or switching speed, further work is suggested which studies the effect of using different structural parameters (e.g., the LC-to-Si composition ratio, or wheel radius and thickness) or different materials (for both LC and semiconductor).

ACKNOWLEDGMENTS

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APPENDIX A: CONSTRUCTION OF LATTICE 2 FROM LATTICE 1

We discuss the construction of the right parallelepiped (cell 2) or its spanning vectors $\{\mathbf{R}_{\parallel}, \mathbf{R}_{\perp 1}, \mathbf{R}_{\perp 2}\}$, for a given propagation direction, e.g., along $\mathbf{k}$ ($\equiv \mathbf{k}/|\mathbf{k}|$, $\mathbf{k}$ being the wave vector). We denote θ_i as the angle between $\hat{\mathbf{k}}$ and $\hat{\mathbf{R}}_i$ ($\equiv \mathbf{R}_i/|\mathbf{R}_i|$), and θ_{ij} as the angle between $\hat{\mathbf{R}}_i$ and $\hat{\mathbf{R}}_j$ (with $\mathbf{R}_i$'s being the primitive lattice vectors of lattice 1). We take $\cos \theta_i$, $\cos \theta_{ij}$, and the ratio $|\mathbf{R}_i|/|\mathbf{R}_j|$ all to be rational numbers. Note that the assumption of rational quantities here does not constrain the general applicability of our model, because, from the computational viewpoint, every real number can be

approximated by a rational one as close as necessary. With the assumption, a lattice vector $\mathbf{R}_{//}$, in the direction of $\hat{\mathbf{k}}$, is constructed, with

$$\mathbf{R}_{//} = N_{//}(\mathbf{R}_1 \frac{\cos \theta_1}{|\mathbf{R}_1|} + \mathbf{R}_2 \frac{\cos \theta_2}{|\mathbf{R}_2|} + \mathbf{R}_3 \frac{\cos \theta_3}{|\mathbf{R}_3|}),$$

where $N_{//}$ is a factor that transforms the coefficients involved here all into integers such that $\mathbf{R}_{//}$ is a lattice vector of lattice 1. It follows that the choice of $\mathbf{R}_{//}$ is not unique. Next, it can be shown, for the vector $\mathbf{R}_{//}$, that one can construct two independent lattice vectors $\mathbf{R}_{\perp 1}$ and $\mathbf{R}_{\perp 2}$ which are both orthogonal to $\mathbf{R}_{//}$. $\mathbf{R}_{\perp 1}$ and $\mathbf{R}_{\perp 2}$ are determined by the orthogonality condition

$$\mathbf{R}_{\perp i} \cdot \mathbf{R}_{//} = 0, \quad i = 1, 2,$$

as follows. Let

$$\mathbf{R}_{\perp i} = \sum_{j=1 \sim 3} n_{ij} \mathbf{R}_j, \quad n_{ij} = \text{integer}.$$

Then, the orthogonality condition yields the following equation for n_{ij} 's,

$$0 = \sum_{j=1 \sim 3} n_{ij} \frac{|\mathbf{R}_j|}{|\mathbf{R}_1|} \sum_{k=1 \sim 3} \cos \theta_k \cos \theta_{jk}, \quad n_{ij} = \text{integer},$$

where the coefficients in the equation are all rational according to our assumption. Upon multiplication by a suitable factor, we can transform the equation into one with integer coefficients

$$0 = \sum_{j=1 \sim 3} n_{ij} m_j, \quad i = 1, 2.$$

This equation determines the coefficients n_{ij} 's in $\mathbf{R}_{\perp 1}$ and $\mathbf{R}_{\perp 2}$. Since these are just two constraints on six variables, there are multiple solutions. For example, a specific solution can be obtained by setting $n_{11} = 0$ and $n_{22} = 0$. This gives $(n_{11}, n_{12}, n_{13}) = (0, m_3, -m_2)$ for $\mathbf{R}_{\perp 1}$ and $(n_{21}, n_{22}, n_{23}) = (m_3, 0, -m_1)$ for $\mathbf{R}_{\perp 2}$. Together with $\mathbf{R}_{//}$, they span a right parallelepiped unit cell for the given propagation direction $\hat{\mathbf{k}}$.

APPENDIX B: CONNECTIONS BETWEEN RECIPROCAL LATTICE 1 AND RECIPROCAL LATTICE 2

As mentioned, reciprocal lattice 1 is a subset of reciprocal lattice 2. Therefore, a vector $\mathbf{G}$ of reciprocal lattice 1 can be written as the linear combination

$$\mathbf{G} = n_{//} \mathbf{G}_{//}^{(0)} + (n_{\perp 1} \mathbf{G}_{\perp 1}^{(0)} + n_{\perp 2} \mathbf{G}_{\perp 2}^{(0)}),$$

where $\{\mathbf{G}_{//}^{(0)}, \mathbf{G}_{\perp 1}^{(0)}, \mathbf{G}_{\perp 2}^{(0)}\}$ as defined in the text are the primitive lattice vectors of reciprocal lattice 2. We make the identification

$$\begin{aligned} \mathbf{G}_{//} &= n_{//} \mathbf{G}_{//}^{(0)}, \\ \mathbf{G}_{\perp} &= n_{\perp 1} \mathbf{G}_{\perp 1}^{(0)} + n_{\perp 2} \mathbf{G}_{\perp 2}^{(0)}, \end{aligned}$$

which confirms the statement in the text that the projections $\mathbf{G}_{//}$ and $\mathbf{G}_{\perp}$ belong to reciprocal lattice 2. The expansion coefficients $n_{//}$, $n_{\perp 1}$, and $n_{\perp 2}$ in the above are integers subject to some constraint to be derived in the following.

We write alternatively $\mathbf{G} = n_1 \mathbf{G}_1 + n_2 \mathbf{G}_2 + n_3 \mathbf{G}_3$, where $\mathbf{G}_i$'s as defined in the text are the primitive lattice vectors of reciprocal lattice 1, and n_1 , n_2 , and n_3 are integers (with no constraint). The condition on $n_{//}$, $n_{\perp 1}$, and $n_{\perp 2}$ is determined by the equation

$$n_{//} \mathbf{G}_{//}^{(0)} + n_{\perp 1} \mathbf{G}_{\perp 1}^{(0)} + n_{\perp 2} \mathbf{G}_{\perp 2}^{(0)} = n_1 \mathbf{G}_1 + n_2 \mathbf{G}_2 + n_3 \mathbf{G}_3. \quad (\text{B1})$$

$\{n_{//}, n_{\perp 1}, n_{\perp 2}\}$ can be solved in terms of $\{n_1, n_2, n_3\}$, if we transform, in Eq. (B1), $\{\mathbf{G}_{//}^{(0)}, \mathbf{G}_{\perp 1}^{(0)}, \mathbf{G}_{\perp 2}^{(0)}\}$ on the l.h.s. into $\{\mathbf{G}_1, \mathbf{G}_2, \mathbf{G}_3\}$ and then equate the corresponding coefficients of $\mathbf{G}_i$'s on both sides. The transformation is determined by that between $\{\mathbf{R}_{//}, \mathbf{R}_{\perp 1}, \mathbf{R}_{\perp 2}\}$ and $\{\mathbf{R}_1, \mathbf{R}_2, \mathbf{R}_3\}$,

$$\begin{pmatrix} \mathbf{R}_{//} \\ \mathbf{R}_{\perp 1} \\ \mathbf{R}_{\perp 2} \end{pmatrix} = S \begin{pmatrix} \mathbf{R}_1 \\ \mathbf{R}_2 \\ \mathbf{R}_3 \end{pmatrix}, \quad S \equiv (s_{ij}),$$

where s_{ij} 's are all integers and determined in Appendix A. In terms of s_{ij} 's, the transformation between $\{\mathbf{G}_{//}^{(0)}, \mathbf{G}_{\perp 1}^{(0)}, \mathbf{G}_{\perp 2}^{(0)}\}$ and $\{\mathbf{G}_1, \mathbf{G}_2, \mathbf{G}_3\}$ is given below

$$\begin{aligned} \mathbf{G}_{//}^{(0)} &= \frac{1}{|\det(S)|} \sum_{ijk} s_{2i} s_{3j} \varepsilon_{ijk} \mathbf{G}_k, \\ \mathbf{G}_{\perp 1}^{(0)} &= \frac{1}{|\det(S)|} \sum_{ijk} s_{3i} s_{1j} \varepsilon_{ijk} \mathbf{G}_k, \\ \mathbf{G}_{\perp 2}^{(0)} &= \frac{1}{|\det(S)|} \sum_{ijk} s_{1i} s_{2j} \varepsilon_{ijk} \mathbf{G}_k. \end{aligned} \quad (\text{B2})$$

In the case of a cubic structure, as considered in our work, we have the following volume ratio

cell 1 (spanned by $\{\mathbf{R}_1, \mathbf{R}_2, \mathbf{R}_3\}$): cell 2 (spanned by $\{\mathbf{R}_{//}, \mathbf{R}_{\perp 1}, \mathbf{R}_{\perp 2}\}$) = $|\det(S)|$: 1. In general, $|\det(S)| > 1$, since cell 2 is typically larger than cell 1.

Substituting Eq. (B2) into Eq. (B1) yields the transformation

$$\begin{pmatrix} n_{//} \\ n_{\perp 1} \\ n_{\perp 2} \end{pmatrix} = S \begin{pmatrix} n_1 \\ n_2 \\ n_3 \end{pmatrix}, \quad (\text{B3})$$

which expresses $\{n_{//}, n_{\perp 1}, n_{\perp 2}\}$ in terms of $\{n_1, n_2, n_3\}$, thus furnishing the constraint in discussion. Although n_1 , n_2 , and n_3 are arbitrary integers, $\{n_{//}, n_{\perp 1}, n_{\perp 2}\}$ are generally not. This is obviously so in the case where $|\det(S)| > 1$.

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